Controlling material properties using a thermostat

Christoph Junghans

Max Planck Institute for Polymer Research
Mainz

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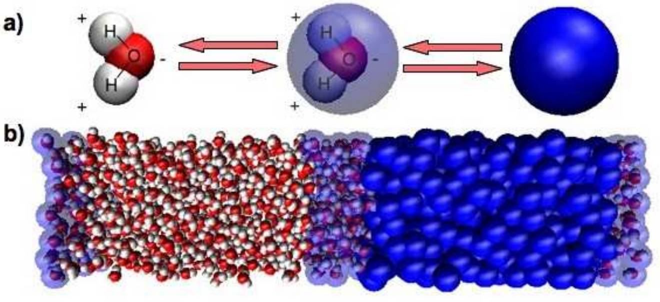
Outline

Motivation

Changing of material properties is useful for:

- Fitting models to real experiments
- Multiscale simulations (AdResS, QMM, etc.)



[1]

[1] From: M. Praprotnik, S. Matysiak, L. Delle Site, K. Kremer and C. Clementi, J. Phys. Condens. Matter 19, 292201, 2007.

Newton's Equation of Motion

$$m\ddot{\vec{r}}_i = \underbrace{\vec{F}_i}_{\text{Deterministic part}} \overbrace{+ \underbrace{\vec{F}_i^D}_{\text{Damping part}} + \underbrace{\vec{F}_i^R}_{\text{Random part}}}^{\text{Langevin Thermostat}}$$

Ensemble: NVE

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Ensemble: NVT

Dissipative Particle Dynamics (DPD) Thermostat [2]

Advantages of DPD

- Local thermostat
- Galilei invariant
- Satisfies Newton III
- Conservation → Hydrodynamics
  - Mass
  - Momentum
  - Angular momentum
- Does not influence the dynamics very much

[2] T. Soddemann, B. Dünnweg, and K. Kremer (2003)

DPD Equations I

Damping and random force

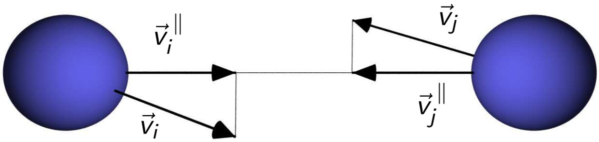
$$\vec{F}_i^{\mathrm{D}} = \sum_{j \neq i} \vec{F}_{ij}^{\mathrm{D}} \quad \text{and} \quad \vec{F}_i^{\mathrm{R}} = \sum_{j \neq i} \vec{F}_{ij}^{\mathrm{R}}$$

with

$$\vec{F}_{ij}^{\mathrm{D}} = -\zeta(r_{ij})(\hat{r}_{ij} \otimes \hat{r}_{ij})\vec{v}_{ij}$$

and

$$\vec{F}_{ij}^{\mathrm{R}} = \sigma(r_{ij})\hat{r}_{ij}\theta_{ij}$$



DPD Equations I

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Choice of the projector

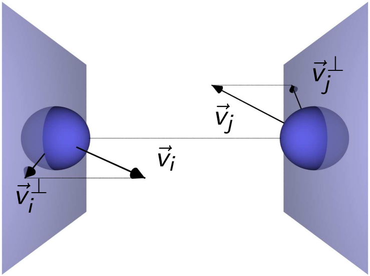
Interesting cases

- Standard DPD

$$\overleftrightarrow{P}_{ij} = \hat{r}_{ij} \otimes \hat{r}_{ij}$$

- Transverse DPD

$$\overleftrightarrow{P}_{ij} = \overleftrightarrow{I} - \hat{r}_{ij} \otimes \hat{r}_{ij}$$



Focker-Planck-Equation and Temperature

Study of the Focker-Planck-Equation leads to:

Fluctuation-dissipation theorem

$$\sigma(r)^2 = \zeta(r) k_B T$$

We chose:

Weighting function

$$\zeta(r) = \zeta \Theta(r - r_{cutoff})$$

Lennard-Jones fluid

Setup

- 4000 particles
- Purely repulsive Lennard-Jones interaction

$$U_{\mathrm{LJ}} = 4\epsilon \left(\frac{1}{r^{12}} - \frac{1}{r^{6}} + \frac{1}{4} \right)$$

- $r_{\mathrm{cutoff}} = 2^{1/6}$
- Different DPD thermostats at $T_{\mathrm{input}} = 1.2$
- $\rho_N = N/V = 0.8638$
- Varying friction strength ζ and thermostats

Lennard-Jones fluid

Basic observables

- Temperature

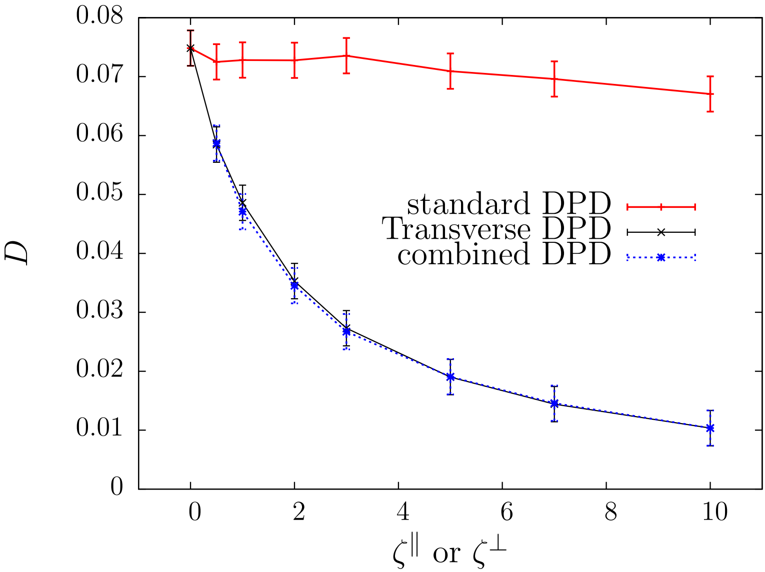
$$T = \frac{2E_{\text{kin}}}{3N_{\text{part}}} = 1.2 \pm 0.01$$

- Pressure

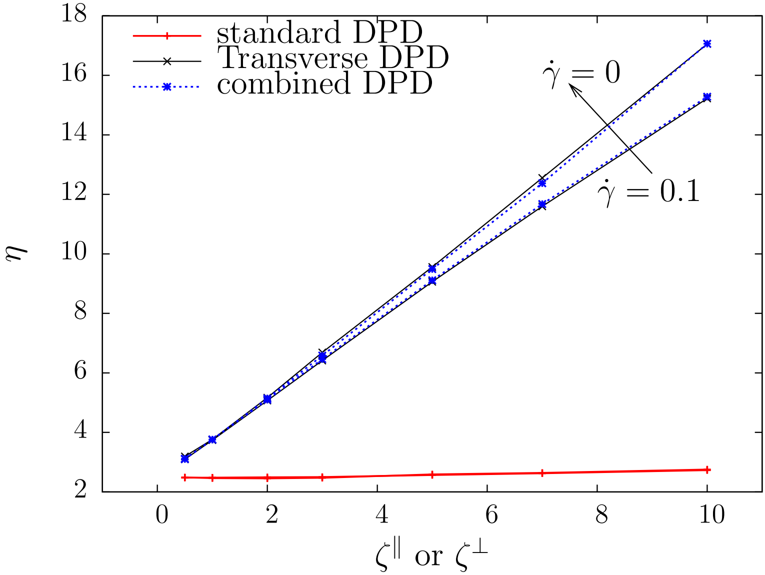
$$p = 9.8 \pm 0.2$$

- Radial distribution function ✓

Lennard-Jones fluid
Diffusion constant



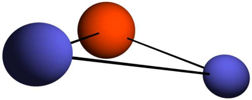
Lennard-Jones fluid
Viscosity



TIP3P water and coarse-grained water

Setup

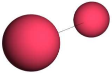
TIP3P water model



Rigid bonds

$$\zeta^{\parallel} = 0.038\mathrm{ps}^{-1}$$
$$\zeta^{\perp} = 0.000\mathrm{ps}^{-1}$$

Coarse-grained model



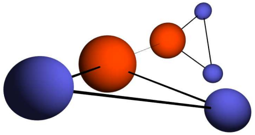
Tabulated potential

$$\zeta^{\parallel} = 0.00\mathrm{ps}^{-1}$$
$$\zeta_1^{\perp} = 0.50\mathrm{ps}^{-1}$$
$$\zeta_2^{\perp} = 0.75\mathrm{ps}^{-1}$$
$$\zeta_3^{\perp} = 1.00\mathrm{ps}^{-1}$$

TIP3P water and coarse-grained water

Setup

TIP3P water model



Lennard-Jones

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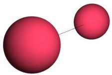
Coarse-grained model



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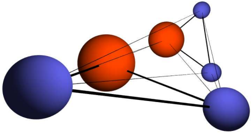
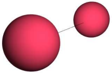


Coulomb

$\zeta^{\parallel} = 0.038 \text{ps}^{-1}$
$\zeta^{\perp} = 0.000 \text{ps}^{-1}$

Coarse-grained model



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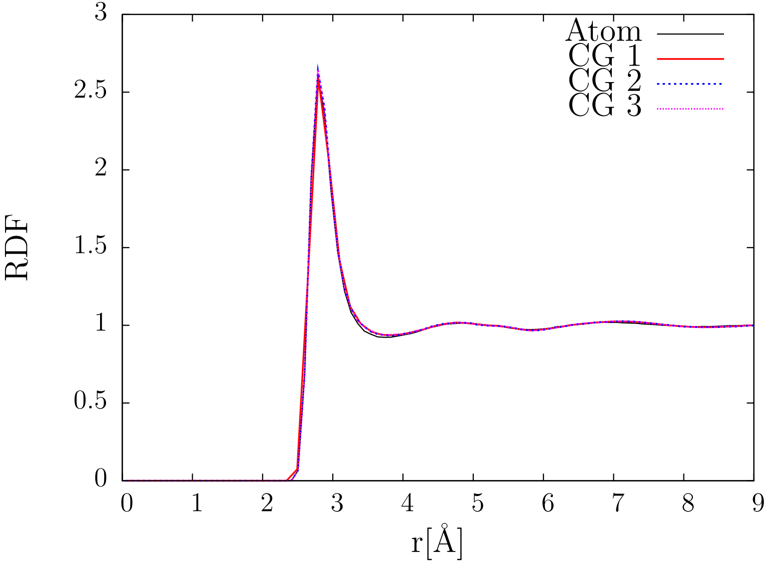
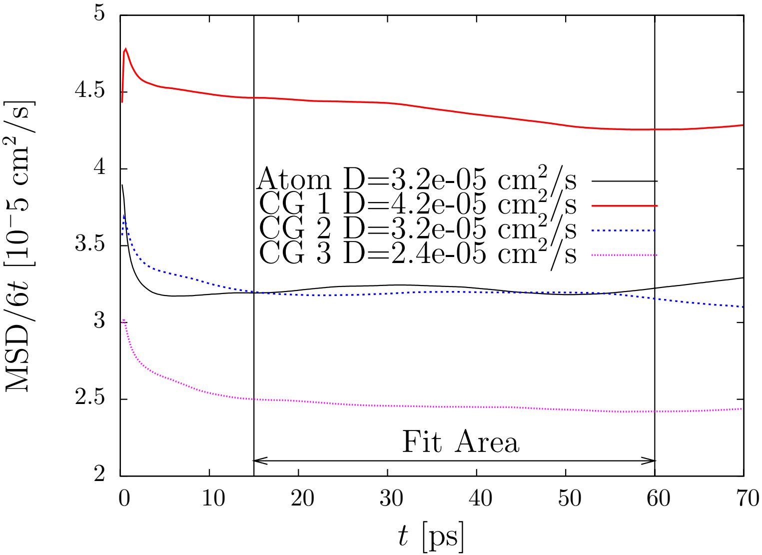
TIP3P water and coarse-grained water

RDF



TIP3P water and coarse-grained water
Diffusion constant



TIP3P water and coarse-grained water

Other observables

- Temperature

$$T = \frac{2E_{\text{kin}}}{3N_{\text{part}}} = 300 \pm 0.5\text{K}$$

- Diffusion constant $(D = 3.2\text{cm}^2/s)$ matches at:

$$\zeta^{\perp} = 0.75ps^{-1}$$

- Viscosity $(\eta = 0.5 \cdot 10^{-3}\text{Pa} \cdot \text{s})$ matches at:

$$\zeta^{\perp} = 0.6ps^{-1}$$

Conclusion

- Simple method to tune timescale of NVT simulations
- Analytical studies with Mori-Zwanzig formalisms show similar behaviour
- Extension to mass dependent version
- Implemented in ESPResSo package[3]
- Further details see: "*Transport properties controlled by a thermostat: An extended dissipative particle dynamics thermostat*" [4]

[3] www.espresso.mpg.de

[4] CJ, M. Praprotnik and K. Kremer, Soft Matter (2008)

The End

Thank you for your attention !